

Dimensional effects in ultrathin magnetic films

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Dimensional effects in the critical properties of multilayer Heisenberg films have been numerically studied by Monte Carlo methods. The effect of anisotropy created by the crystal field of a substrate has been taken into account for films with various thicknesses. The calculated critical exponents demonstrate a dimensional transition from two-dimensional to three-dimensional properties of the films with an increase in the number of layers. A spin-orientation transition to a planar phase has been revealed in films with thicknesses corresponding to the crossover region.

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I. INTRODUCTION

Great attention has been recently focused on studying the properties of thin magnetic films [1] primarily because the investigation of the physical properties of ferromagnetic films promotes the solution to fundamental problems in the physics of magnetic phenomena and the development of the theory of ferromagnetism [2]. Study of thin films significantly expands concepts of the physical nature of the anisotropy of ferromagnets and makes it possible to reveal diverse remagnetization processes and to observe new physical phenomena [3]. Structural states that can hardly be obtained in bulk samples can be implemented in films. This significantly expands the possibilities of the study of the relation between the structural characteristics and physical properties of magnetic materials.

Study of the physical properties of thin ferromagnetic films is also topical for their technological applications. The most important application of films is their use as magnetic media for writing and storage of information in memory devices. Features of magnetic films can promote an increase in the information writing density to 1 TBit/in² [4]. In this respect, it is very important to understand processes of variation of magnetization in thin magnetic films with change in the temperature, particularly at temperatures close to the Curie temperature.

The critical properties of ultrathin films are sensitive to effects of anisotropy created by the critical field of a substrate. These effects can be responsible for change in the critical behavior of multilayer systems.

In this work, the physical properties of thin ferromagnetic films are numerically studied within the anisotropic Heisenberg model with the Hamiltonian [5]

$$H = -J \sum_{i,j} [(1 - \Delta(N)) (S_i^x S_j^x + S_i^y S_j^y) + S_i^z S_j^z], \quad (1)$$

where $\mathbf{S}_i = (S_i^x, S_i^y, S_i^z)$ is the three-dimensional unit vector at the i th site, $J > 0$ characterizes the ferromagnetic exchange interaction between nearest spins, and Δ is the

anisotropy parameter. The values $\Delta = 0$ and 1 correspond to the isotropic Heisenberg model and Ising model, respectively.

The microscopic nature of anisotropy in Fe, Co, and Ni films and its dependence on the thickness of a film measured in the number of monoatomic layers N are determined by the crystal field of the substrate, single-ion anisotropy, and dipole-dipole interaction between the magnetic moments of atoms in the film and their mutual competition. For this reason, the calculation of the anisotropy effects in magnetic films is very difficult. The effective dependence of the anisotropy parameter $\Delta(N)$ on the thickness of the film N is chosen proportional to the N dependence of the critical temperature for Ni(111)/W(110) films [6] with different numbers of layers. In the approximation procedure for the dependence $\Delta(N)$, we used the fact that Ni films with a large number of layers exhibit bulk critical properties corresponding to three-dimensional isotropic Heisenberg magnets [7, 8]. The resulting dependence $\Delta(N)$ is shown in Fig. 1.

The Monte Carlo simulation was performed for $L \times L \times N$ films with periodic boundary conditions in the plane of the film. The number of spins in each layer is

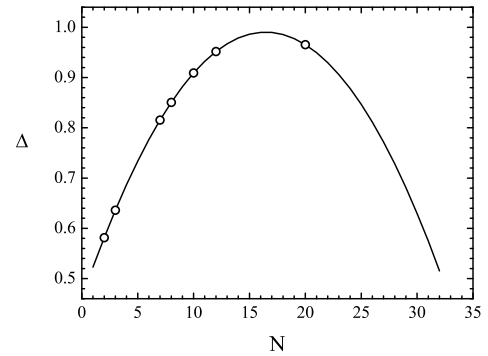


FIG. 1: Anisotropy parameter $\Delta(N)$ versus the thickness of the film N . The circles are experimental data for Ni(111)/W(110) [6].

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$L \times L$ and the number of layers in the thin film is N . In this work, we considered systems with linear dimensions $L = 32, 48$, and 64 and the number of layers ranging from $N = 1$ to 32 . The characteristics of the film were calculated for the temperature interval $T = 0.01 - 5.01$ with a step $\Delta T_{\text{step}} = 0.02$.

Within the three-dimensional anisotropic Heisenberg model with the use of the SwendsenWang algorithm, we studied the temperature dependencies of the magnetization

$$m = \left\langle \frac{1}{N_s} \left[\sum_{\alpha \in \{x,y,z\}} \left(\sum_i^{N_s} S_i^\alpha \right)^2 \right]^{1/2} \right\rangle, \quad (2)$$

its components, i.e., the magnetization normal to the plane of the film

$$m_z = \left\langle \frac{1}{N_s} \sum_i^{N_s} S_i^z \right\rangle, \quad (3)$$

and the magnetization in the plane of the film

$$m_{xy} = \left\langle \frac{1}{N_s} \left[\left(\sum_i^{N_s} S_i^x \right)^2 + \left(\sum_i^{N_s} S_i^y \right)^2 \right]^{1/2} \right\rangle, \quad (4)$$

as well as the orientational order parameter [7, 8]

$$O_\alpha = \left\langle \left| \frac{n_h^\alpha - n_v^\alpha}{n_h^\alpha + n_v^\alpha} \right| \right\rangle, \quad (5)$$

Here, $N_s = NL^2$ is the total number of spins in the film, angular brackets mean statistical averaging, $\alpha \in \{x, y, z\}$, and n_h and n_v are the numbers of the horizontal and vertical pairs of nearest spins with oppositely directed S_z , respectively:

$$\begin{aligned} n_h^\alpha &= \sum_{\mathbf{r}} \left\{ 1 - \text{sgn} [S^\alpha(r_x, r_y), S^\alpha(r_x + 1, r_y)] \right\}, \\ n_v^\alpha &= \sum_{\mathbf{r}} \left\{ 1 - \text{sgn} [S^\alpha(r_x, r_y), S^\alpha(r_x, r_y + 1)] \right\}. \end{aligned} \quad (6)$$

The critical behavior of the system near the phase-transition temperature is clearly characterized by the magnetic susceptibility

$$\chi_m \sim [\langle m^2 \rangle] - [\langle m \rangle]^2. \quad (7)$$

The dependence $\chi_m(T)$ characterizes critical fluctuations of the magnetization and their interaction. The temperature at the maximum of the temperature dependence $\chi_m(T)$ can be used to estimate the temperature of a ferromagnetic phase transition in the film and its dimensional changes for various thicknesses of the film.

The temperature behavior of the orientational susceptibility

$$\chi_o \sim [\langle O_\alpha^2 \rangle] - [\langle O_\alpha \rangle]^2. \quad (8)$$

makes it possible to reveal the region of the spin-orientation transition from a phase in which the magnetization is normal to the plane of the film to a phase where the magnetization preferentially orients in the plane of the film.

To more accurately determine the critical temperature of the transition from the paramagnetic phase to the ferromagnetic one, we found the temperature dependence of the Binder cumulant:

$$U_4(T, L) = \frac{1}{2} \left(3 - \frac{[\langle m^4(T, L) \rangle]}{[\langle m^2(T, L) \rangle]^2} \right). \quad (9)$$

The scaling dependence of the cumulant

$$U_4(T, L) = u \left(L^{1/\nu} (T - T_c) \right). \quad (10)$$

allows determining the temperature of a second-order phase transition from the coordinate of the intersection of the temperature dependencies $U_4(T, L)$ for different L values.

In this work, we considered the finite-dimensional scaling form [9] in films for the quantities

$$\begin{aligned} \langle m(T, N) \rangle &= L^{-\beta/\nu} \tilde{m}(L^{1/\nu} \tau, N) \\ \chi_m(T, N) &= L^{\gamma/\nu} \tilde{\chi}(L^{1/\nu} \tau, N) \end{aligned} \quad (11)$$

where γ , β , and ν are the effective critical exponents of the susceptibility χ_m , magnetization m , and correlation length ξ , respectively. Scaling form (11) determines the dependence of m and χ_m on the linear dimension L and the number of the layers N in the film and makes it possible to determine the effective critical exponents from the resulting temperature dependencies of these quantities. The detailed analysis of the behavior of the magnetizations m , m_{xy} , and m_z and the susceptibilities χ_m and χ_o for films with various thicknesses revealed two types of phase transitions. A transition from the ferromagnetic phase to the paramagnetic one is observed for all N values under consideration. The indicated transition is accompanied by a peak of the magnetic susceptibility χ_m . These magnetizations and susceptibilities for films with $N = 1$ and 9 are shown in Fig. 2. According to the data shown in Fig. 2a, although m_z vanishes in the region of the phase transition temperature, the critical nature of the transition is determined by fluctuations of m_z . This statement for a monolayer film is confirmed by the results reported in [5]. The critical temperatures of the ferromagnetic phase transition were determined more accurately by the method of intersection of Binder cumulants (9).

For the interval of the thicknesses of films $N = 9 - 22$, an additional peak in the high-temperature region appears in the dependence $\chi_m(T)$ owing to the spin-orientation transition whose nature is confirmed by the behavior of the orientational susceptibility χ_o . The behavior of the magnetizations m , m_{xy} , and m_z and the susceptibilities χ_m and χ_o for $N = 9$ is shown in Fig. 2b.

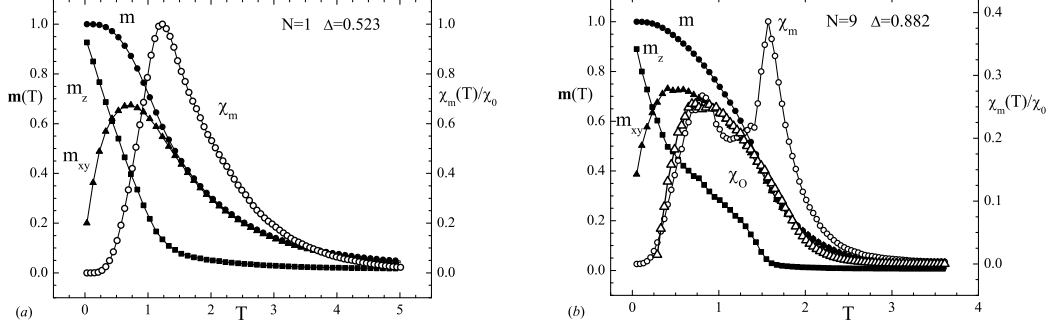


FIG. 2: Temperature dependencies of the magnetizations $m(T)$, $m_z(T)$, and $m_{xy}(T)$ and susceptibilities $\chi_m(T)$, $\chi_0(T)$ for the number of layers $N = 1$ (a) and 9 (b).

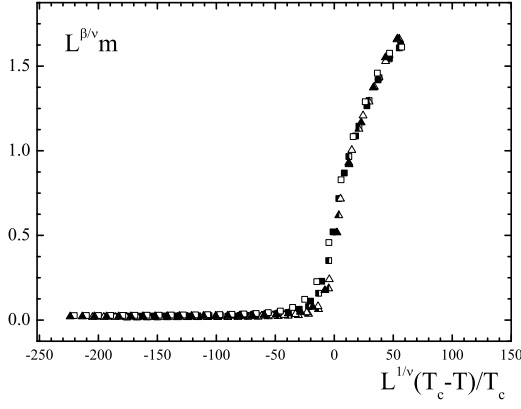


FIG. 3: Scaling dependence $f(m) = L^{\beta/\nu} m$ versus $L^{1/\nu}(T_c - T)/T_c$.

The specification of the critical behavior of the film to a certain universality class, as well as the effective dimension of the system, can be characterized by a set of critical exponents. The critical exponent ν can be determined from the scaling behavior of Binder cumulants (9), and the critical exponents β/ν and γ/ν can be found from scaling dependencies (11) of the magnetization m and susceptibility χ on L at the corresponding critical temperature T_c .

The scaling dependencies $f(m) = L^{\beta/\nu} m$ on $L^{1/\nu}(T_c - T)/T_c$ calculated for films with the linear dimensions $L = 32, 48$, and 64 and thicknesses from 2 to 5 ML exhibit collapse of the data (Fig. 3) on a single universal curve. This confirms that the effective critical exponents are calculated correctly.

The analysis of the temperature dependencies of the model quantities for various numbers of layers in the film N shows that they are separated into several groups with different asymptotic critical behaviors. In particular, films with the number of layers $N < 5$ exhibit a

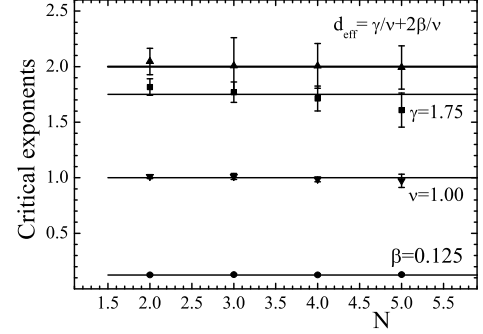


FIG. 4: Critical exponents ν , β , γ and effective dimension d_{eff} .

behavior with critical exponents close to the exact values for the two-dimensional Ising model ($\beta_{2\text{DIsing}} = 1/8$, $\nu_{2\text{DIsing}} = 1$, $\gamma_{2\text{DIsing}} = 7/4$; Fig. 4): $\beta = 0.126(8)$, $\nu = 1.010(17)$, and $\gamma = 1.816(69)$ at $N = 2$; $\beta = 0.128(8)$, $\nu = 1.011(27)$, and $\gamma = 1.770(94)$ at $N = 3$; $\beta = 0.126(9)$, $\nu = 0.986(21)$, and $\gamma = 1.713(112)$ at $N = 4$; and $\beta = 0.129(9)$, $\nu = 0.972(59)$, and $\gamma = 1.609(150)$ at $N = 5$. Using the hyperscaling relation $\gamma/\nu + 2\beta/\nu = d$, the effective dimension of the system d_{eff} can be obtained. For films with the thickness $N = 2 - 5$, d_{eff} is close to 2 (see Fig. 4). Thus, the films with $N/L \ll 1$ exhibit the critical behavior characteristic of quasi-two-dimensional systems. The resulting critical exponent $\beta(N)$ presented in Fig. 5 clearly exhibits the transition from the behavior of the two-dimensional Ising model to the three-dimensional Heisenberg model with an increase in the thickness of the film. The dimensional transition demonstrated in this work from two-dimensional to three-dimensional critical properties of multilayer magnetics with an increase in the thickness of the film is in good agreement with the experimental data (see Fig. 2 in [6] and Fig. 7 in [1]).

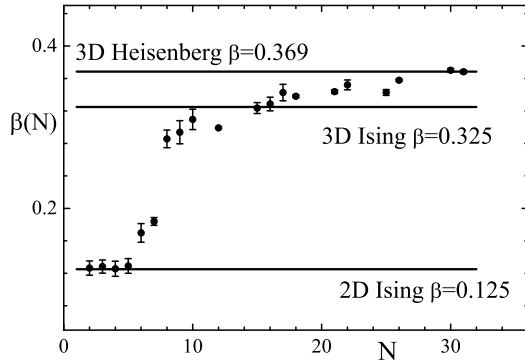


FIG. 5: Critical exponent β versus the thickness of the film N .

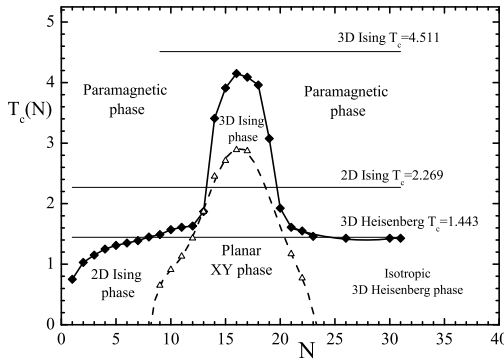


FIG. 6: Phase diagram for thin films. The solid line corresponds to the transition from the ferromagnetic phase to the paramagnetic phase and the dashed line corresponds to the spin-reorientation transition.

Figure 6 shows the resulting phase diagram of change in the state of thin-film systems with an increase in their thickness. The systems with $N \leq 5$ exhibit the critical behavior corresponding to the two-dimensional Ising model. The critical behavior of films with $6 \leq N \leq 12$ corresponds to the crossover region of the transition from two-dimensional properties to three-dimensional ones. The critical characteristics for films with the thicknesses $N = 13 - 21$ correspond to the three-dimensional Ising model. In films with $9 \leq N \leq 22$, the spin-reorientation transition occurs to the planar phase with the critical behavior close to the behavior of the XY model. Since the planar phase is revealed, it is necessary to significantly

expand the necessary set of data at the statistical averaging of the calculated quantities. Films with $N \geq 22$ exhibit the bulk critical behavior corresponding to an isotropic Heisenberg magnet. The results are confirmed by the critical exponents presented in the table.

To summarize, the numerical investigation of the magnetic properties and critical behavior of thin films within the anisotropic Heisenberg model has revealed dimensional effects in the behavior of the magnetization and

TABLE I: Critical exponents β , ν and γ

	β	ν	γ
$N = 2 \div 5$	0.127(2)	0.995(10)	1.727(45)
2D Ising model	0.125	1.0	1.750
$N = 6$	0.170(11)	0.974(62)	1.803(76)
8	0.286(11)	0.981(28)	1.586(52)
10	0.310(13)	0.839(32)	1.225(61)
$N = 15$	0.324(7)	0.632(21)	1.141(33)
16	0.329(8)	0.634(28)	1.182(53)
17	0.343(10)	0.658(27)	1.132(42)
3D Ising model [12]	0.3249(6)	0.6299(5)	1.2331(13)
$N = 26$	0.358(1)	0.723(18)	1.396(121)
31	0.368(2)	0.759(40)	1.414(77)
3D Heisenberg model [13]	0.3685(11)	0.710(2)	1.393(4)

magnetic susceptibility. A spin-reorientation transition has been identified in films with the thicknesses $N = 9 - 22$ ML. The critical exponents β , ν , and γ have been calculated for films with various thicknesses. The resulting averaged critical exponent $\gamma = 1.73(5)$ for $N \leq 5$ is in good agreement with the experimental value $\gamma = 1.75(2)$ measured for a Fe/W(110) bilayer film in [14]. A transition from the two-dimensional to three-dimensional properties in the behavior of multilayer magnets with an increase in the thickness of the film has been revealed for the first time.

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